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LETTER TO THE EDITOR

Localisation in disordered three-dimensional systems

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Abstract. The question of localisation is examined by employing a significant improved localisation function method. Results are presented for the localisation function $L(E)$ and its upper limit function $L^*(E)$ for a simple cubic-lattice tight binding model with zero disorder. We find, in contrast to the two-dimensional case, that $L(E)$ is clearly larger than 1 (except of course at the end of the band) and that $L^*(E)$ is almost equal to $L(E)$. Thus a critical amount of disorder must be exceeded before the localisation sets in. Furthermore $L^*(E)$, which is easier to calculate, is a reasonable approximation to $L(E)$.

Recently Soukoulis and Economou (1980), using a significantly improved localisation function method $L(E)$ (Economou and Cohen 1970, 1972, Licciardello and Economou 1975), demonstrated that for a periodic two-dimensional (2D) lattice the true $L(E)$ inside the band is equal to 1 within numerical uncertainties. As the disorder increases from zero, one expects that $L(E) < 1$ for all E, implying that all states are localised in a 2D system with non-zero disorder in agreement with recent scaling theories (Abrahams *et al* 1979). On the other hand, the upper limit function $L^*(E)$, which is calculated within the strong-correlations assumption (Economou and Cohen 1970, 1972), is much higher than $L(E)$. The big difference between $L^*(E)$ and $L(E)$ in a 2D system suggests that the localisation of eigenstates in the weak disorder limit is due to long-range multiple-scattering effects which produce very slowly decaying states. Numerical work in finite samples (Weaire and Kramer 1980) indicates that 'localised' states appear only when the disorder exceeds a critical value which is approximately given by $L^*(E) = 1$. This led us to conjecture that $L^*(E) \leqslant 1$ implies strong localisation, while $L(E) < 1 < L^*(E)$ implies very weak localisation which is not revealed in the numerical work.

The purpose of this Letter is to report results for $L(E)$ and $L^*(E)$ for a periodic 3D system. These results show, in contrast to the 2D case, that $L(E)$ is clearly larger than 1 (except of course at the end of the band) and that $L^*(E)$ is almost equal to $L(E)$. Thus a critical amount of disorder must be exceeded before localisation sets in. Furthermore $L^*(E)$, which is easier to calculate, is a reasonable approximation to $L(E)$.

The localisation function $L(E)$ which is less (more) than 1 in the regions of the spectrum consisting of localised (propagating) eigenstates is given by

$$L(E) = \lim_{N\to\infty} \left| \sum_j V^{N+1} t_j^{(N)}(E) \right|^{1/N} \tag{1}$$

where V is the off-diagonal matrix elements V_{ij} of the tight binding Hamiltonian (Ander-

son 1958)

$$H = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_j V_{ij} |i\rangle\langle j|$$

and

$$t_j^N \equiv G_{n_1}^0 G_{n_2}^{0,\,n_1} \cdots G_{n_2}^{0,\,n_2\,\cdots\,n_{N-1}} = \det\{G_j^N\}/G_{00} \tag{2}$$

where

$$G_{n_i}^{0,n_1\cdots} = \langle n_i | (z - H^{0,n_1\cdots})^{-1} | n_i \rangle. \tag{3}$$

The superscripts $0, n_1 \ldots$ denote that $\varepsilon_0 = \varepsilon_{n_1} = \ldots = \infty$. The summation over j in equation (1) is over the set of all sites $n_1, n_2 \ldots n_N$ which form self-avoiding paths starting and ending at site 0. The t_j^N in equation (2) was expressed (Soukoulis and Economou 1980) as a determinant of Green's functions with no sites excluded. $G_{nm} = \langle n | (z - H)^{-1} | m \rangle$, where the sites n and m belong to the self-avoiding path. In the present case of zero disorder, G_{nm} are the periodic Green's functions, which can be calculated very accurately. We also define the quantity $L^*(E)$ as

$$L^*(E) = \lim_{N\to\infty} \left[\sum_j |t_j^{(N)}(E)| \right]^{1/N}. \tag{4}$$

Clearly $L^*(E) \geqslant L(E)$. The equality holds for E at the band edge (or outside it). The assumption of strong correlations (Economou and Cohen 1970, 1972) puts $L^*(E) = L(E)$. It was shown by Soukoulis and Economou (1980) that the strong-correlations assumption is not valid for a periodic 2D lattice. Taking into account that $(M_N)^{1/N} \to K$ as $N \to \infty$, where M_N is the total number of self-avoiding polygons and K is the connectivity of the lattice ($K = 4.6826$ for the cubic lattice), we can write

$$L^*(E) = KV \lim_{N\to\infty} \langle |t_j^{(N)}(E)| \rangle^{1/N} \tag{5}$$

where the angular brackets indicate the average overall j of order N. We have calculated the quantity $\langle |t_j^{(N)}(E)| \rangle^{1/N}$ up to $N = 8$ by evaluating explicitly $\det\{G_j^N\}$ for all the self-avoiding closed paths (polygons) up to $N = 8$. The calculations are facilitated because many different paths give (due to symmetry considerations) the same value for $\det\{G_j^N\}$: e.g. to obtain the contribution of the 3312 self-avoiding polygons of the order $N = 8$ one needs to evaluate only 11 distinct determinants of order 8×8. We found that $\langle |t_j^{(N)}(E)| \rangle^{1/N}$ becomes weakly dependent on N as N increases; thus the $N \to \infty$ limit can be obtained rather accurately, as shown in figure 1.

The Green's functions $G_{nm}(E + is)$ for an infinite cubic lattice were calculated by some well known recursion relations (Horiguchi 1971). We were able to calculate G_{nm} with an accuracy up to the seventh significant figure. Details will be presented elsewhere.

In figure 2 we present our results for $L^*(E)$ against E according to the method we described above. A test of the accuracy of our calculation is the behaviour of $L^*(E)$ for $E \geqslant ZV$, where $L^*(E) = L(E)$; $L(E)$ must approach 1 monotonically as $E \to ZV^+$, where $Z = 6$ is the coordination number for the cubic lattice. Figure 2 shows that this is actually the case with a less than 1% numerical uncertainty.

The interesting quantity to calculate is $L(E)$ and not its upper limit $L^*(E)$. To calculate $L(E)$ one needs the Green's functions G_{nm} for real energies. We can obtain them only by considering a finite-size system; then one faces the problem of having large fluctuations in the Green's functions depending on how close the energy E lies on an

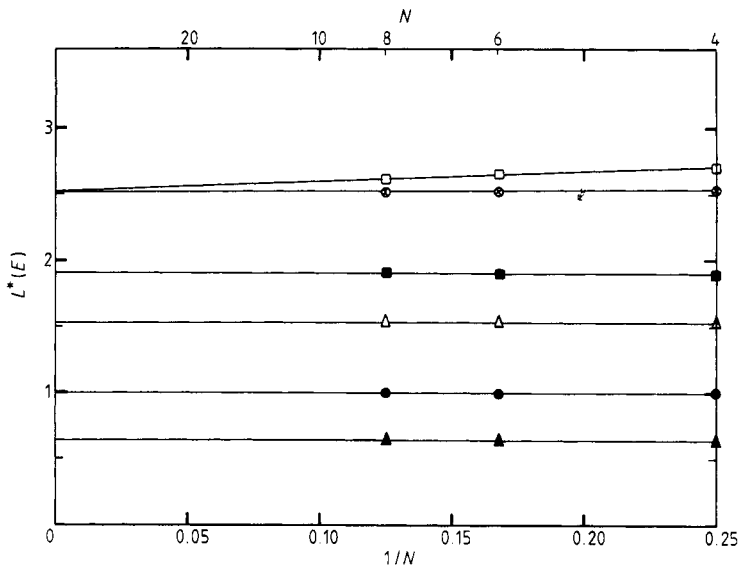

Figure 1. The upper limit $L^*(E)$ of the localisation functions for various energies E is obtained by extrapolating $KV\langle|t_j^{(N)}(E)|\rangle^{1/N}$ to the $1/N = 0$ limit. Values of $E/2V$ are as follows: × 0; ○ 0.5; □ 1.0; ■ 1.5; △ 2.0; ● 3.0; ▲ 4.0.

eigenenergy of the finite system. Of course, in the $N \rightarrow \infty$ limit this problem disappears. To overcome this difficulty which is present in our case because the maximum N we consider is 8, we have applied the following procedure. We generated R random energies inside a narrow energy region around $E(R \simeq 20\text{–}40)$. The results are insensitive to the energy width provided that it is a few times the average level spacing. We only kept

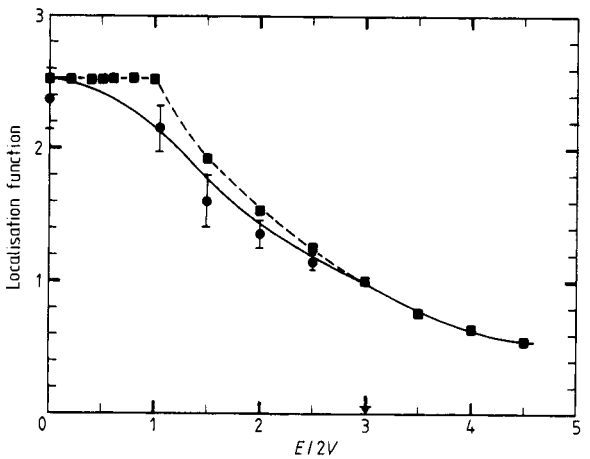

Figure 2. The localisation function $L(E)$ (full curve) and its upper limit $L^*(E)$ (broken curve) against $E/2V$ for a cubic lattice in the limit of infinitesimal disorder. At the band edges ($E = \pm ZV$, where $Z = 6$) $L^*(E) = L(E) = 1$. The full squares represent results for $L^*(E)$ for an infinite-sized system and the full circles are results for $L(E)$ from finite systems; bars indicate estimated errors.

those energies for which $|G_{00}(E)|$ are not higher than two or three times $|G_{00}(E + is)|$ for the infinite periodic lattice. We impose periodic boundary conditions on our periodic finite systems ($13 \times 13 \times 13$, $19 \times 19 \times 19$, $23 \times 23 \times 23$ sites). Having calculated the Green's functions $G_{nm}(E)$ we evaluated—through equation (2)—$t_j^N(E)$ for all self-avoiding polygons up to order 8. We obtained $L(E)$ and $L^*(E)$ by extrapolating to $N \to \infty$ the quantities $KV|\overline{\langle t_j^{(N)}(E)\rangle}|^{1/N}$ and $KV\overline{\langle|t_j^{(N)}(E)|\rangle}^{1/N}$ respectively. The bars indicate logarithmic averages over the R random energies around E. Because we are dealing with finite systems and real energies the errors associated with the $N \to \infty$ extrapolation were significantly larger than in the case of the infinite system for most of the energies inside the band (see figure 2). These errors can be decreased either by calculating self-avoiding polygons of higher order or by increasing the number R of random energies one generates. The results for the finite system were checked by comparing $L^*(E)$ (not shown in figure 2) with the $L^*(E)$ obtained for the infinite system. The agreement is reasonably good. $L(E)$ was found to be a little less than $L^*(E)$ but considerably higher than 2, as one sees in figure 2. It is clear from this work that in the present 3D system $L(E) \simeq L^*(E)$, which implies that the strong-correlations assumption does not introduce significant errors. Furthermore, the results in figure 2 clearly show that a finite amount of disorder is needed to localise all the eigenstates in 3D systems.

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